Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

April 10, 2014

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Pleiades Supercomputer Augmented with New Ivy Bridge Racks

- The HECC Supercomputing Systems team augmented Pleiades' production capacity with 29 new Ivy Bridge racks (2,088 nodes), replacing 20 Nehalem (1,280 nodes) and 12 Westmere racks (768 nodes). A subset of the Nehalem nodes and all of the Westmere nodes will be incorporated into the Merope supercomputer.
- The new Ivy Bridge augmentation increases Pleiades peak performance by 671 teraflops, bringing the overall theoretical peak to 3.6 petaflops and increasing the system's computational capability by 22.9%.
- The new racks were integrated into Pleiades in four phases over a four-month period. Each phase involved hardware installation, software installation, testing, and integration. Each of the first three phases was completed, with racks released into production, in less than two weeks.
- The fourth phase was more challenging due to InfiniBand (IB) issues that impacted the stability of the IB fabric, requiring diagnosis and further testing. The final 7 racks were delivered to the floor during the fourth phase.

Mission Impact: Continued augmentation of the HECC supercomputing environment provides increased computational capability needed to support the increasing requirements of NASA's mission directorates.

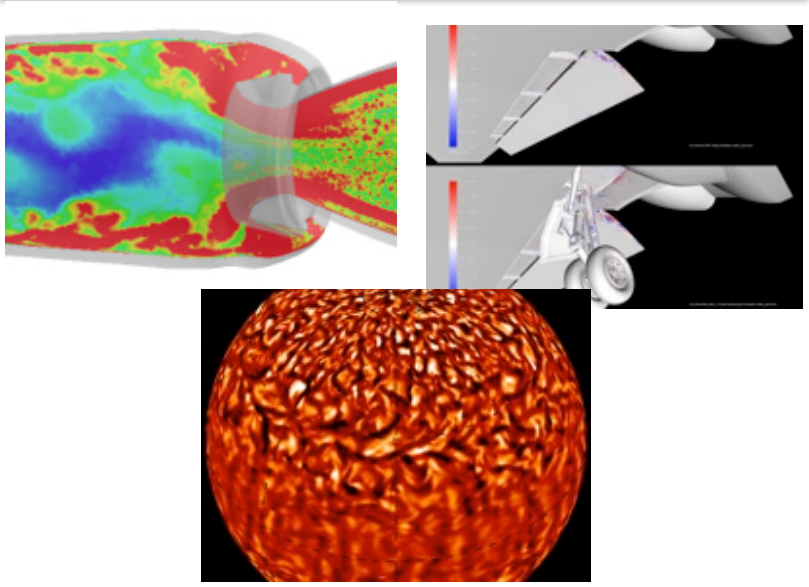
The addition of 29 new Ivy Bridge racks increases Pleiades' computational capability by 22.9%. With the latest augmentation, the system has a total of 163 racks containing 11,176 nodes, with a theoretical peak performance of 3.6 petaflops.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NASA Advanced Supercomputing Division, Computer Science Corp.

March Usage on Pleiades Exceeds 11.5 Million SBUs and Sets New Monthly Record

- March showed record-high usage of the Pleiades supercomputer, with 11.54 million Standard Billing Units (SBUs) used by NASA's science and engineering organizations, exceeding the previous record of 10.74 million SBUs (set in December 2013) by over 7%.
- This increase was enabled by the addition of 2088 Ivy Bridge nodes in the first quarter of 2014 and by efficient operations that delivered 80% system utilization (75% utilization is target).
- The top four projects (from ARMD, HEOMD, SMD, and NESC) each used over 350,000 SBUs during the month and together accounted for 2.76 million SBUs (24%) of the usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA's users.

Mission Impact: Increasing Pleiades' system capacity provides Mission Directorates with more resources for the accomplishment of their goals and objectives.



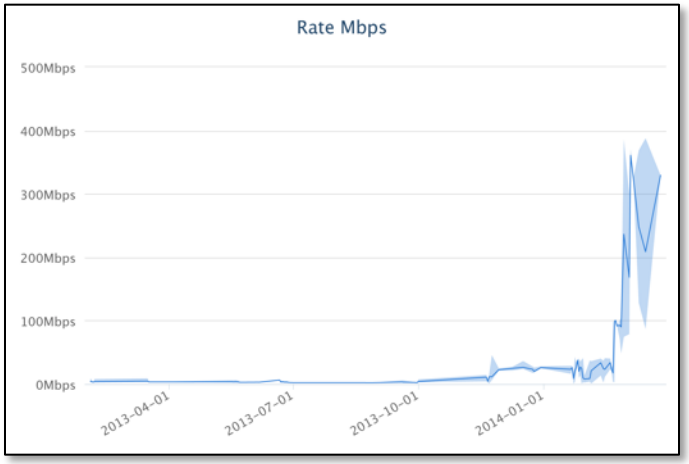
Images representing projects that were among the top users in their respective Mission Directorates. Clockwise from top: 1) Snapshot of the interaction between pressure waves and inhibitors inside the SLS's reusable SRM, HEOMD, H. Yang/J. West. 2) Visualizations of the simulated flow field for a Gulfstream aircraft in landing configuration, ARMD, M. Khorrami; 3) Simulations of global Sun convection, SMD, A. Kosovichev.

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov,
(650) 604-3180, NASA Advanced Supercomputing Division

Network Engineers Help Increase Data Transfer Performance for NOAA User by 80x

- Using in-house flow analysis tools, the HECC Network team was able to identify a user from the National Oceanic and Atmospheric Administration (NOAA) who was getting sub-optimal performance—about 5 megabits per second (Mbps)—while transferring multiple terabytes of data to HECC resources.
- After the team made local routing changes to better manage traffic going to the remote site, the average transfer rate increased 20x (from 5 Mbps to 100 Mbps).
- Further analysis showed that the remote system required tuning for wide area network (WAN) data transfers. HECC engineers contacted the user (Quan Xiao-Wei) and provided tuning instructions for his system. After tuning, his transfer rate from the NAS facility to his system at NOAA increased to about 400 Mbps—for a total improvement of 80x.
- The NOAA site continued to have 1–2% packet loss outbound, so HECC engineers notified their counterparts at NOAA of a local area network problem at their end. NOAA network staff confirmed the problem and are working on a solution.
- Xiao-Wei was very satisfied with the help from HECC network engineers. “Thanks all for your efforts to improve my network connection!”

Mission Impact: By continuously monitoring network performance and optimizing data transfer rates, HECC experts enable scientists to obtain computational results in minutes rather than having to wait hours or days for their results.



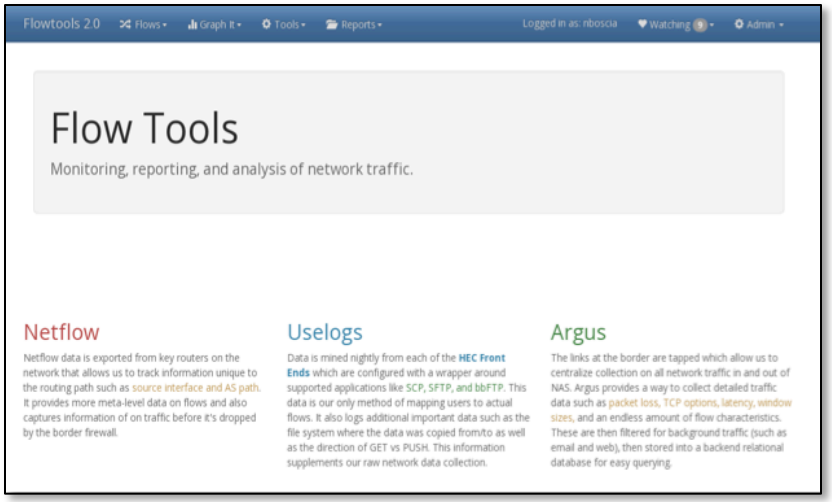
This graph shows the network rate that National Oceanic and Atmospheric Administration (NOAA) users received while transferring data from NOAA to NASA Ames Research Center, before and after the fixes were implemented.

POC: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, NASA Advanced Supercomputing Division, Computer Sciences Corp.

New Version of HECC-Developed Network Data Collection Utility Released

- "Flow Tools," developed by the HECC Network team, is a data collection utility that helps network engineers identify sub-optimal file transfer rates and the users that are affected by the slow performance.
- Network engineers completed an upgrade of the utility to include information that was not available with previous data sources. Flow Tools 2.0 integrates this information with other data sources to improve the data analysis capability for HECC engineering staff.
- New features include:
  - Site searches that allow engineers to determine whether sub-optimal transfer performance relates to one host or an entire site.
  - "ntop" reports (slide 7) are available for one-day, one-week, last 30 days, last quarter, annual, and all-time flow records.
  - A new and improved user interface provides an integrated view of all the additional data HECC now collects. It also allows each network engineer to "like" flows of interest and track them over time.

Mission Impact: The upgraded Flow Tools 2.0 utility improves HECC network engineers' ability to isolate and resolve file transfer performance problems, end-to-end.



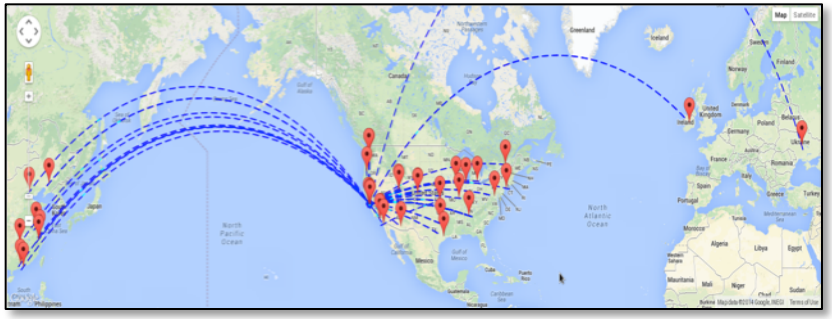
A screenshot of the new and improved web user interface of Flow Tools 2.0, based on the Bootstrap framework.

POC: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Network Team Implements New Real-Time Traffic Visualization Tool

- The HECC Network team implemented a new tool called “ntop,” which enables network engineers to visualize interactions of external traffic in real-time, based on data collected from network taps at the NASLAN border, which interconnects with WAN networks.
- With the new tool, network engineers are able to see data transfers as they occur, including:
  - Duration of data transfer
  - Volume of data transfer
  - Total throughput
  - Real-time impact of route modifications
  - Top *n* data transfers by host
- The ntop tool also provides an active world map of all connections into and out of the NAS facility.

Mission Impact: Implementing new and improved network traffic monitoring tools gives HECC staff the capability to better support the user community, by more efficiently identifying and resolving network performance issues.



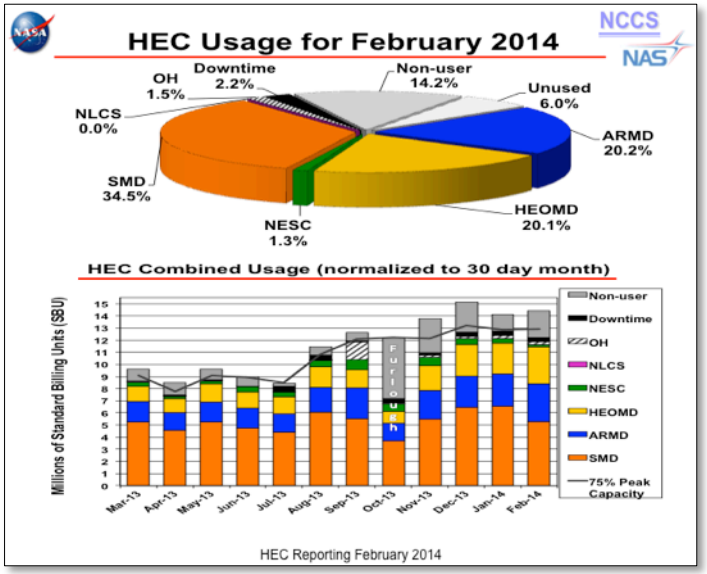
A screenshot of the web-based user interface showing the world map of active connections into the NAS facility.

POC: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Production of HEC Program Monthly Status Reports Transitioned to HECC

- The HECC Tools team worked with NASA Center for Climate Simulation (NCCS) to enhance the High-End Computing (HEC) Program Monthly Status Report production process, which now utilizes a common database and analytics tool for creating spreadsheets and slides for the NAS and NCCS facilities. The HECC team now generates the reports each month.
- The work was enabled by the May 2011 adoption of a common capacity and usage measure (a standard billing unit or SBU) by HECC and NCCS staff.
- The teams' work to generate the 30-chart reports included:
  - Establishing a connection between the two facilities for data transfers, and developing scripts to achieve the daily transfer.
  - Developing common tables for data coming from HECC's Portable Batch System (PBS) and NCCS' Simple Linux Utility for Resource Management (SLURM).
  - Uploading NCCS data since 2011 into MicroStrategy.
  - Developing templates for all reports and charts.
  - Correcting inconsistent formulae and making slides uniform for titles, labels, use of SBUs, and more.
  - Validating data by comparing historic reports and verifying processor information.
- Data coming from PBS and SLURM are now uploaded into the reports database, where they are accessible from MicroStrategy and available for further use.
- Future development includes template improvements, review of new and current charts, and further automation of the reporting process.

Mission Impact: Implementing a consolidated database enables NASA's HEC Program Monthly Status Reports to provide consistent data across the program, and makes the data readily available for further use.



The High-End Computing Program Monthly Status Report consists of 30 charts covering the usage and capacity of the supercomputing systems at the NASA Advanced Supercomputing facility and NASA Center for Climate Simulation.

POCs: Elizabeth Hartman, blaise.hartman@nasa.gov, (650) 604-2539, NASA Advanced Supercomputing (NAS) Division, Bay Systems Inc.; Ryan Spaulding, ryan.c.spaulding@nasa.gov, (408) 772-6567, NAS Division, ADNET Systems

Apple's OS X 10.9 Mavericks Being Deployed to HECC Staff

- To stay ahead of the technology curve, HECC's Engineering Servers and Services (ESS) team developed a Mavericks image for Mac systems used by scientific staff in the NASA Advanced Supercomputing (NAS) facility.
- Once the image passed a NAS security scan and was approved by the NASA Ames Exploration Technology Directorate's security official, the ESS team began deploying it on NAS systems.
- Preparation work for the Mavericks image included:
  - Developing the Casper process to build the image and install all default and selected applications.
  - Upgrading Tecplot, Mathematica, Matlab and Fieldview to the latest versions and testing all HECC/NAS applications.
  - Configuring security settings, system defaults and FileVault for the system.
  - Acquiring and setting up Symantec Antivirus to run locally until the agency version is ready.
  - Testing several scenarios for reducing the upgrade time.
- Due to the requirement for a complete rebuild of every Mac, each upgrade takes about one full day. This includes a full backup, system imaging, applications installation, system encryption, data restoration, and preventive maintenance.
- About 180 supported Macs will be upgraded over the next several months. The Mavericks system will allow HECC to run the latest hardware from Apple, including the redesigned Mac Pro, which will be shipping soon.

Mission Impact: Development and approval of an OS X 10.9 Mavericks image enables HECC to support the latest Mac workstations and laptops requested by local scientific users and support staff.

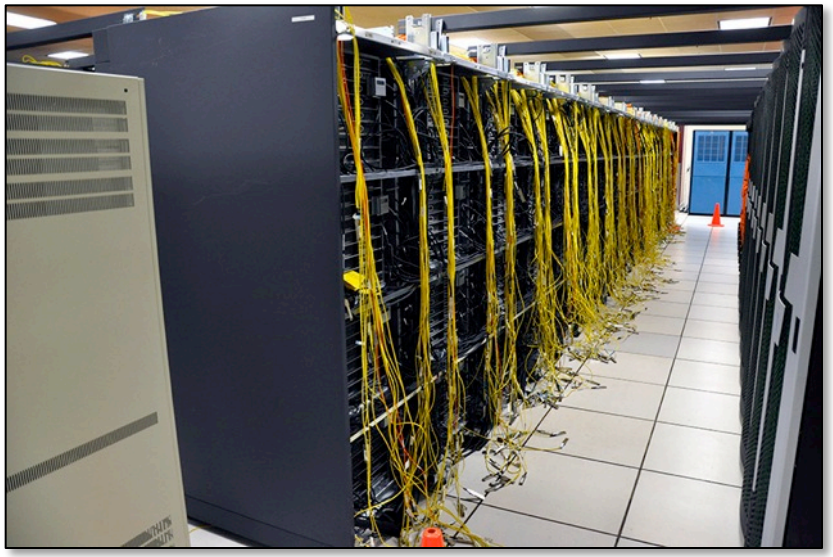
Apple's OS X 10.9 (Mavericks) system was released in October 2013, and is required for the latest MacBook Pro laptops and the new Mac Pro.

POCs: Brooks Patton, brooks.patton@nasa.gov, (650) 604-3967; Sam Fike, sam.g.fike@nasa.gov, (650) 604-1338, NASA Advanced Supercomputing Division, ADNET Systems.

HECC Property Management Accomplishments in 2013

- Property custodians responsible for HECC/NAS property currently track over 1,100 pieces of decaled equipment with a value of over $90M. Each piece of equipment requires numerous updates through its life cycle.
- Equipment management activities for 2013 included:
  - Successfully completing the 2013 annual inventory.
  - Disposing of 104 pieces of tagged equipment with an original value of over $20.3M.
  - Acquiring and tagging 115 pieces of new equipment.
  - Resolving 542 Remedy user tickets for property management activities.
  - Tracking disk removal or data destruction for disposed equipment containing NASA data.
  - Completing hundreds of property forms for equipment ownership, property passes, excess and cannibalization of equipment, and location changes.
- The Property staff's active tracking and updating of HECC/NAS equipment helps ensure a successful annual inventory, and prepares for a smooth application of the new radio frequency identification (RFID) asset tags during FY14.

Mission Impact: Accurate tracking of assets through their life cycle at NASA's largest supercomputing facility, and tracking of data removal during system disposal, ensures good control of government equipment and prevents loss of NASA data.



HECC property custodians track the acquisition, movement, and disposal of all NAS facility decaled equipment, including Pleiades supercomputer components.

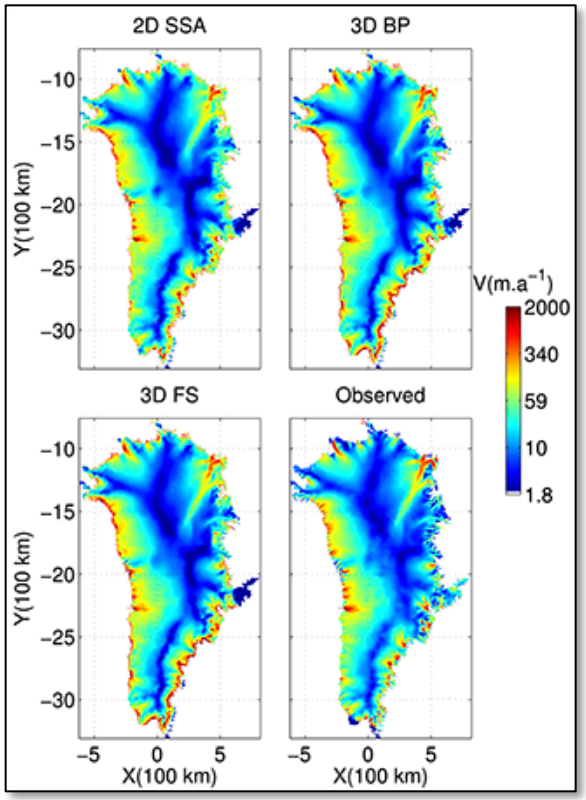
POCs: Judy Kohler, judy.j.kohler@nasa.gov, (650) 604-4303; Chacky Tsan, chacky.s.tsan@nasa.gov, (650) 604-6401, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Pleiades Enables Unique Simulations for Improved Predictions of Sea Level Rise *

- Researchers at the Jet Propulsion Laboratory (JPL) are running simulations on Pleiades and using the Ice Sheet System Model (ISSM) to model and predict the evolution of polar ice caps in Greenland and Antarctica over the next 20–100 years.
- ISSM is a finite element, multi-model, multi-scale framework that is capable of:
  - Modeling the evolution of polar ice sheets at high resolution (1 kilometer, 40 vertical layers).
  - Understanding the sensitivities and uncertainties associated with such predictions, using automatic differentiation and uncertainty analysis.
  - Assimilating NASA observations such as surface altimetry and surface velocities, using adjoint-based optimization to infer properties of the ice sheet, such as basal friction or depth-averaged viscosity.
- Running full Navier-Stokes models would be computationally prohibitive. Using an in-house simplified model that reduces ice flow physics complexity, the JPL team can run simulations of about 5 million degrees of freedom on Pleiades for uncertainty analysis, using about 1,000 processors for 5 days per run.

** HECC provided supercomputing resources and services in support of this work*

Mission Impact: Ice Sheet System Model simulations, enabled by the Pleiades supercomputer, have resulted in unique science pertaining to the stability of polar ice sheets in a changing climate.



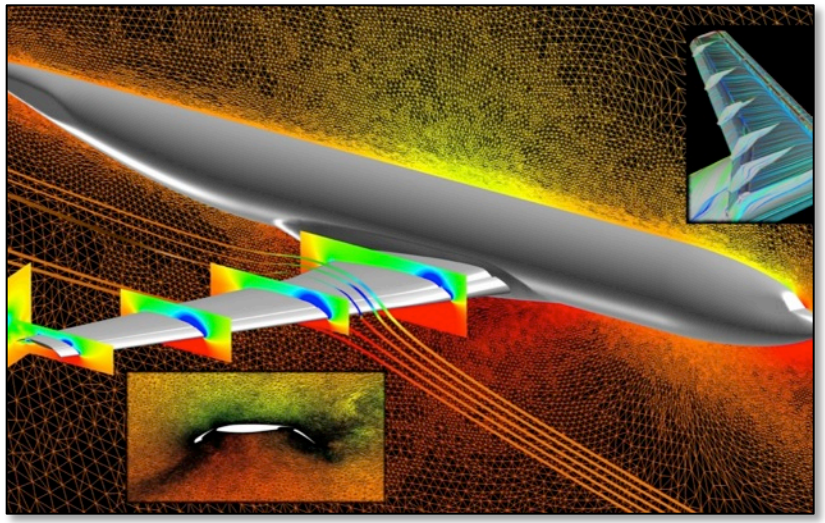
Shown here are results from an Ice Sheet System Model (ISSM) simulation of basal friction at the ice/bed interface under the Greenland Ice Sheet. Model runs included: A 2D collapsed model (2D SSA); a 3D collapsed model (3D BP); and a 3D full Navier-Stokes model (3D FS). Melting polar ice sheets (Antarctica and Greenland) are one of the main contributors to sea level rise.

POC: Eric Larour, eric.larour@jpl.nasa.gov, (818) 970-8032, Jet Propulsion Laboratory

HECC Supports FUN3D Development for Complex Aerospace Design & Analysis *

- To meet the agency's complex aerodynamic challenges, researchers at NASA Langley Research Center are using HECC resources to actively develop FUN3D, a widely used computational fluid dynamics (CFD) toolset that incorporates a comprehensive range of speed regimes and multidisciplinary effects.
- Current projects that use FUN3D include:
  - NASA aeronautics research such as fixed- and rotary-wing vehicles and sonic boom mitigation.
  - Design and analysis of NASA's new Space Launch System, re-entry deceleration concepts, and commercial crew spacecraft development.
  - Efficient green energy concepts such as wind turbine design and drag minimization for long-haul trucking.
- FUN3D simulations use billions of simultaneous equations that can be efficiently solved only with high-performance computing (HPC) resources, such as Pleiades and Endeavour.

Mission Impact: The NASA-developed CFD software suite FUN3D provides the world's foremost adjoint-based design capability. Enabled by HECC resources, FUN3D simulations are used to tackle the agency's most complex aerodynamics problems.



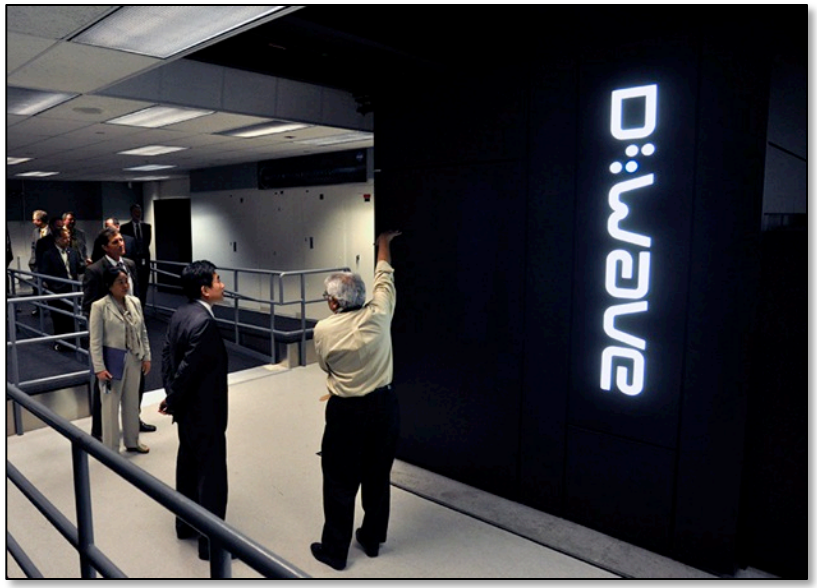
Snapshot from a FUN3D simulation of a transport aircraft in a high-lift configuration, run on the Pleiades supercomputer. FUN3D's adjoint-based adaptation implicitly targets areas of the domain that are critical to accurate lift prediction. The toolset also enables formal adjoint-based design optimization of time-dependent moving-body simulations involving turbulent flows.

POC: Eric Nielsen, eric.j.nielsen@nasa.gov, (757) 864-2239, NASA Langley Research Center

** HECC provided supercomputing resources and services in support of this work*

HECC Facility Hosts Several Visitors and Tours in March 2014

- HECC hosted 10 tour groups in March; guests learned about the agency-wide missions being supported by Pleiades, and viewed scientific results on the hyperwall system. Visitors this month included:
  - NASA Administrator Charlie Bolden visited the NAS facility and was briefed by Rama Nemani, principal scientist on the NASA Earth Exchange (NEX) project.
  - NASA Associate Administrator for Aeronautics Research Mission Directorate (ARMD) Jaiwon Shin visited Ames to roll out the budget, and was briefed by Rupak Biswas at the Quantum Artificial Intelligence Laboratory (QuAIL) on quantum computing technologies for possible ARMD-relevant applications.
  - Professor Rolf Henke (executive board member of the DLR German Aerospace Center), Jaiwon Shin, and other NASA ARMD executives, met with NAS managers to survey computational fluid dynamics research activities in the NAS Division, especially in the area of aerospace technology.
  - A group from the UltraSat Team, including members from the Jet Propulsion Laboratory and Israel's Weizmann Institute, met with NASA management to discuss the status of the proposed mission (which is focused on Earth imaging) and possible HECC collaboration.



Piyush Mehrotra (far right), chief of the NASA Advanced Supercomputing Division, points to the D-Wave system to Jaiwon Shin (second from right), Associate Administrator for Aeronautics Research Mission Directorate (ARMD), who visited NAS along with other senior ARMD executives.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers and Presentations

- "**Shock Waves and Cosmic Ray Acceleration in the Outskirts of Galaxy Clusters**," S. E. Hong, D. Ryu, H. Kang, R. Cen, arXiv:1403.1420 [astro-ph.CO], March 6, 2014. * *http://arxiv.org/abs/1403.1420*
- "**Estimation of Forest Aboveground Biomass in California Using Canopy Height and Leaf Area Index Estimated from Satellite Data**," G. Zhang, S. Ganguly, R. Nemani, et al., Remote Sensing Enviroment (Elsevier), March 11, 2014. * *http://www.sciencedirect.com/science/article/pii/S0034425714000558*
- "**Turbulence-Induced Relative Velocity of Dust Particles II: The Bidisperse Case**," L. Pan, P. Padoan, J. Scalo, arXiv:1403.3865 [astro-ph.EP], March 16, 2014. * *http://arxiv.org/abs/1403.3865*
- "**Temporal Self-Organization in Galaxy Formation**," R. Cen, arXiv:1403.5265 [astro-ph.GA], March 20, 2014. * *http://arxiv.org/abs/1403.5265*
- "**Supporting 'Big Data Analysis and Analytics at the NASA Advanced Supercomputing (NAS) Facility**," P. Mehrotra, L. H. Pryor, F. R. Bailey, M. Cotnoir, NAS Technical Report NAS-2014-02, published online March, 2014. * *http://www.nas.nasa.gov/assets/pdf/papers/NAS_Technical_Report_NAS-2014-02.pdf*

** HECC provided supercomputing resources and services in support of this work*

Papers and Presentations (Continued)

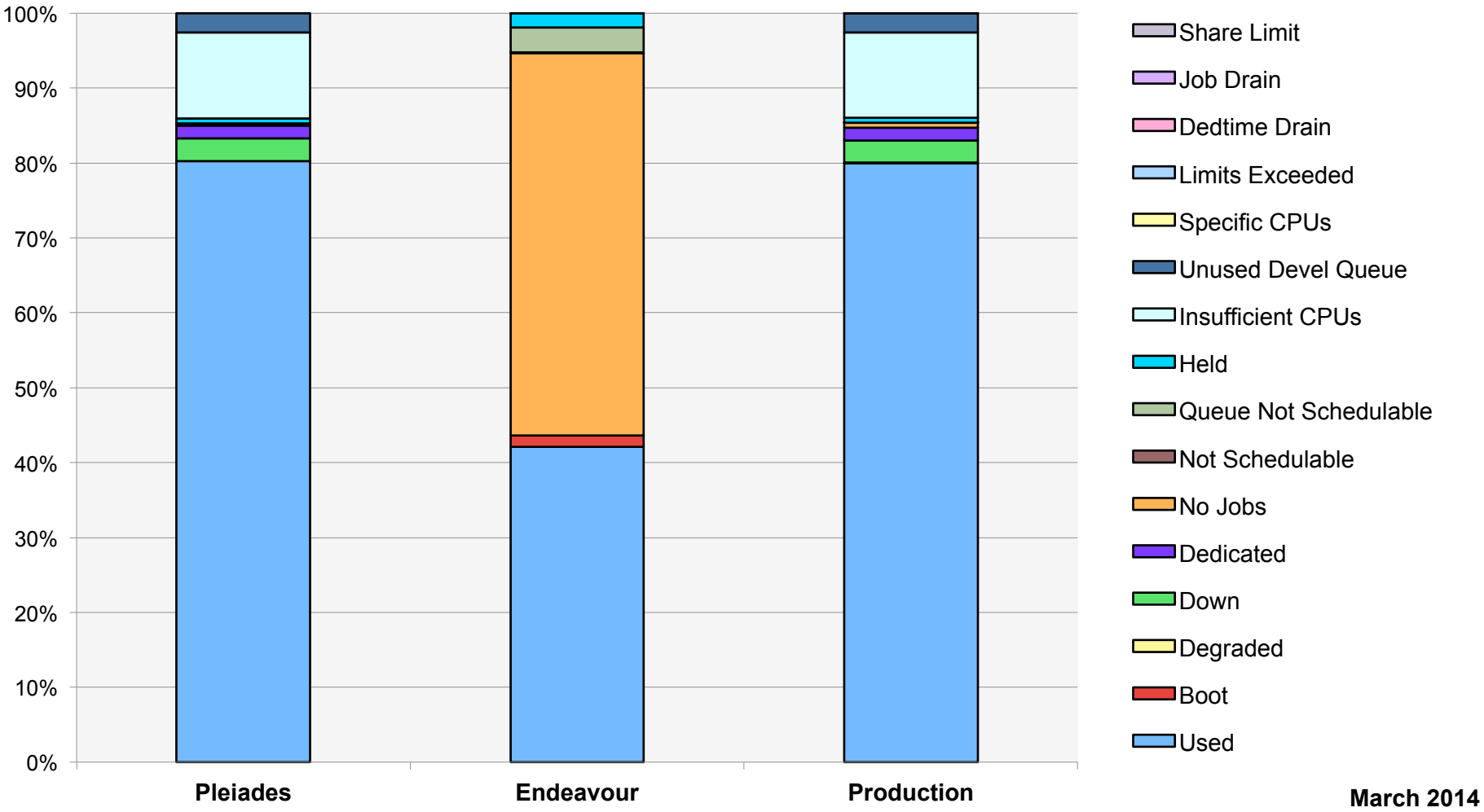
- "**Frequent Spin Reorientation of Galaxies Due to Local Interactions**," R. Cen, arXiv:1403.5274 [astro-ph.GA], March 20, 2014. * *http://arxiv.org/abs/1403.5274*
- "**Particle Acceleration and Magnetic Field Generation in Shear-Flows**," K.-I. Nishikawa, High Energy Phenomena in Relativistic Outflows (HEPRO IV), International Journal of Modern Physics: Conference Series, vol. 28, March 21, 2014. * *http://www.worldscientific.com/doi/pdf/10.1142/S2010194514601951*
- "**Supporting Science at NAS: HPC, Data Analysis and Collaboration**," P. Mehrotra, Conference on Computational Astrophysics 2014-2020: Approaching Exascale, Lawrence Berkeley Lab, March 22, 2014.
- "**HECC – Meeting NASA's High End Computing Goals through Innovation**," W. Thigpen, SGI Worldwide All Hands, March 26, 2014.

** HECC provided supercomputing resources and services in support of this work*

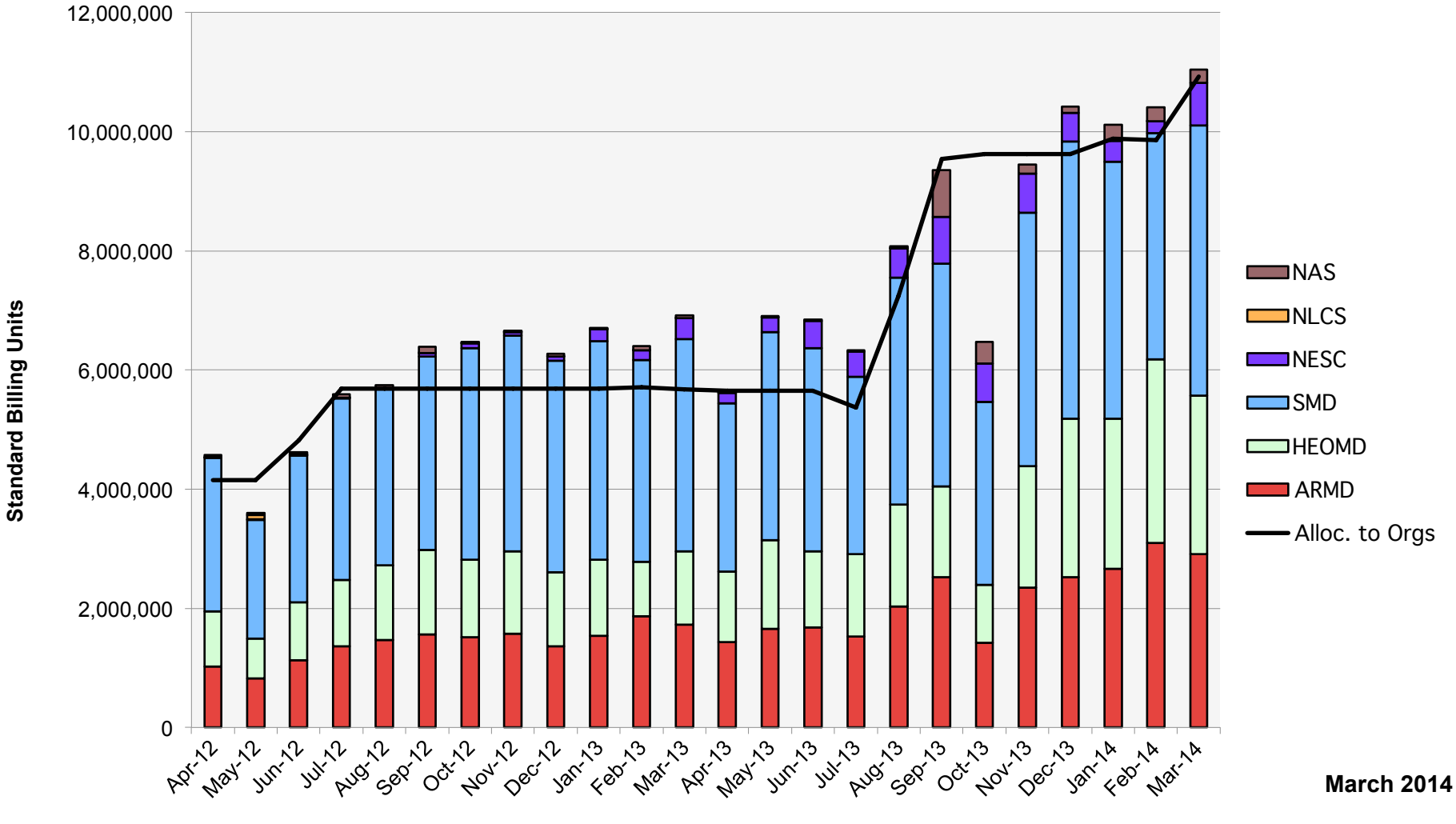
News and Events

- **Regional Nuclear War Would Still Wreak Global Climate Havoc, Says Study**, *Forbes*, March 8, 2014—A study (led by atmospheric scientists at the National Center for Atmospheric Research) published in the journal *Earth's Future* discusses the hypothetical result of nuclear war on Earth's climate, using seven Earth system model simulations run on the Pleiades supercomputer.
  http://www.forbes.com/sites/brucedorminey/2014/03/08/regional-nuclear-war-would-still-wreak-global-climate-havoc-says-study/
- **Photo of the Week: Pi + NASA + Supercomputing**, *Energy.gov (U.S. Department of Energy)*, March 14, 2014—The U.S. Department of Energy featured the NASA Advanced Supercomputing Division's photo of Pleiades as the Photo of the Week on the DOE website, in celebration of Pi-Day (March 14, or 3.14), and displayed as the cover image on their Facebook page. The image was posted on the NAS Flickr page and linked to from the @NASA_NAS Twitter page.
  http://energy.gov/articles/photo-week-pi-nasa-supercomputing
- **Quantum Rewrites the Rules of Computing**, *Computerworld*, March 18, 2014—Computerworld's Sharon Gaudin takes a look at the new field of quantum computing and talks to some of the companies and experts who are leading the charge, including HECC's Rupak Biswas, who discusses NASA's Quantum Artificial Intelligence Lab.
  http://www.computerworld.com/s/article/9247011/Quantum_rewrites_the_rules_of_computing

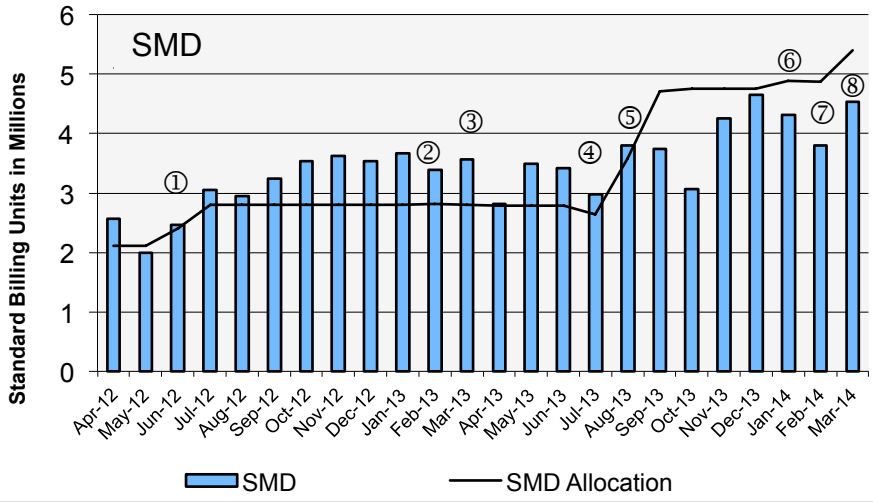
HECC Utilization

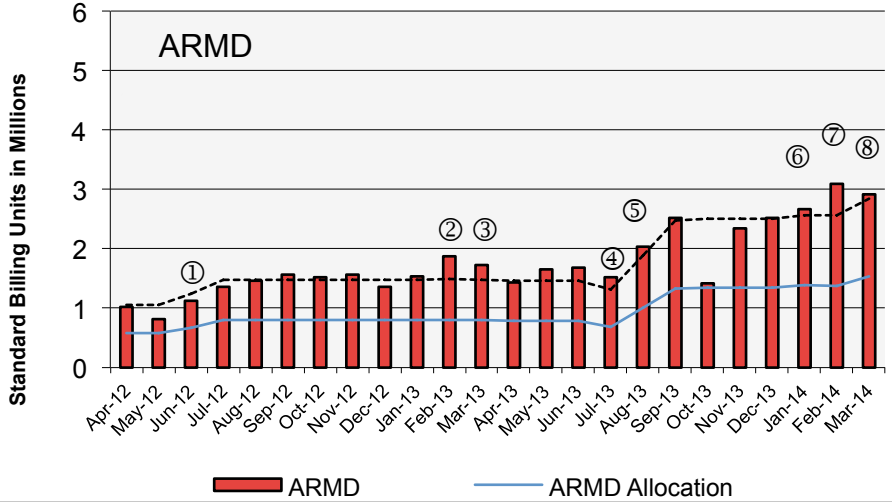


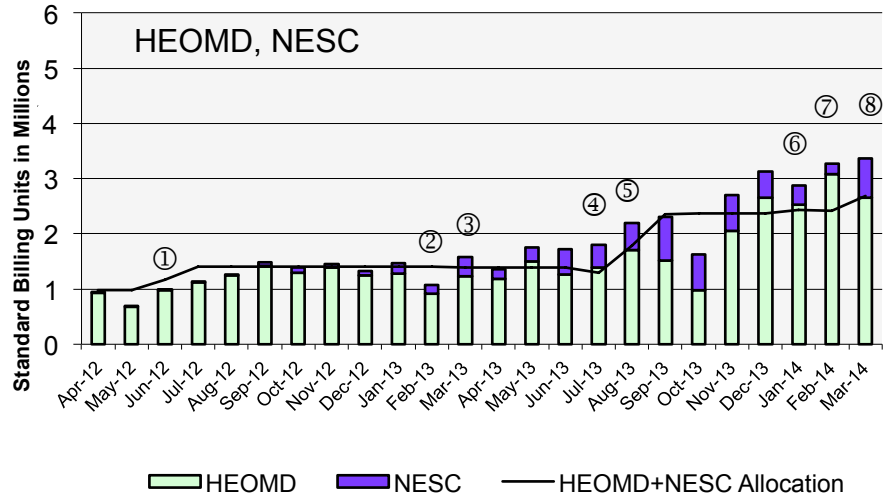
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month

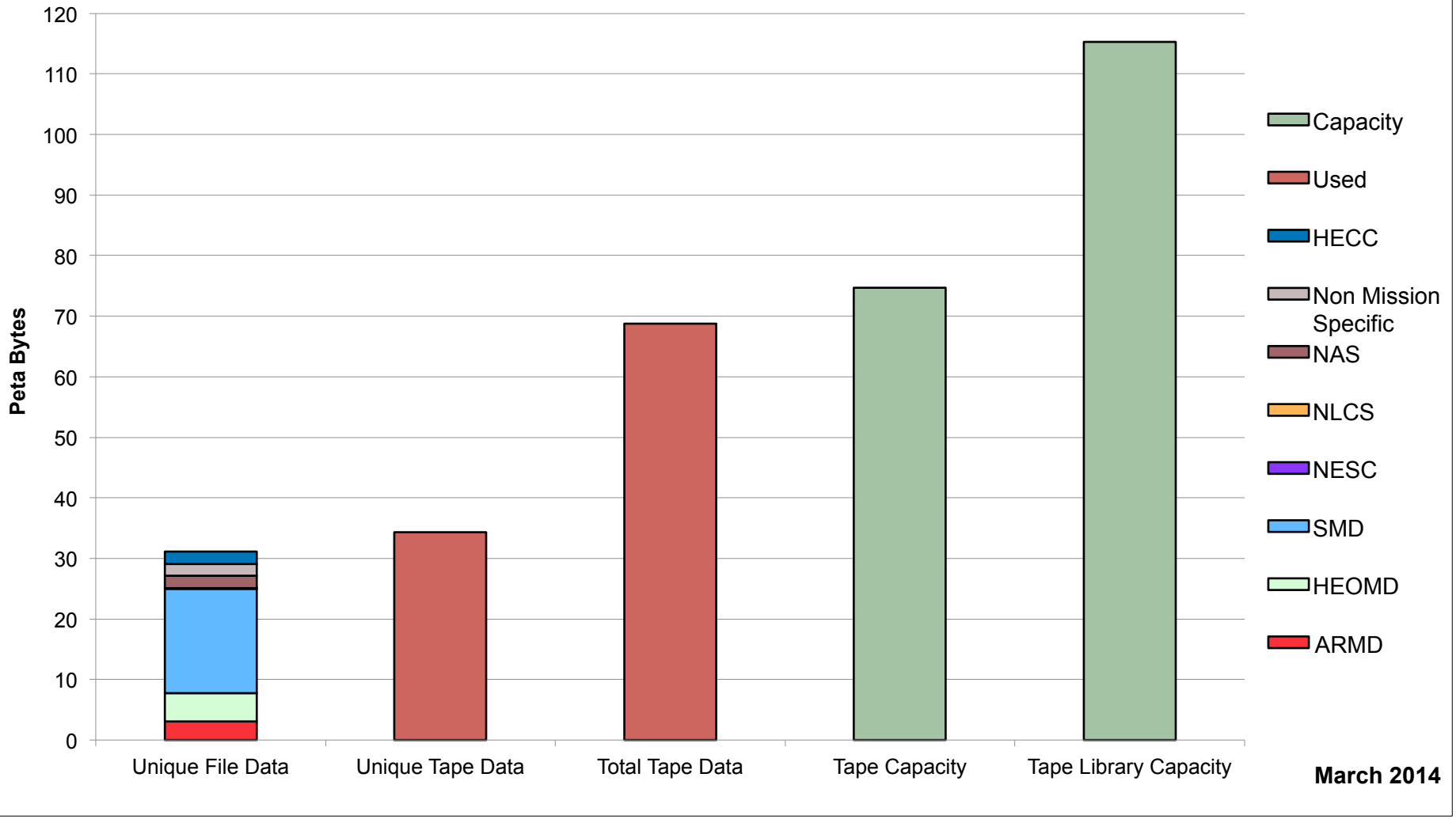




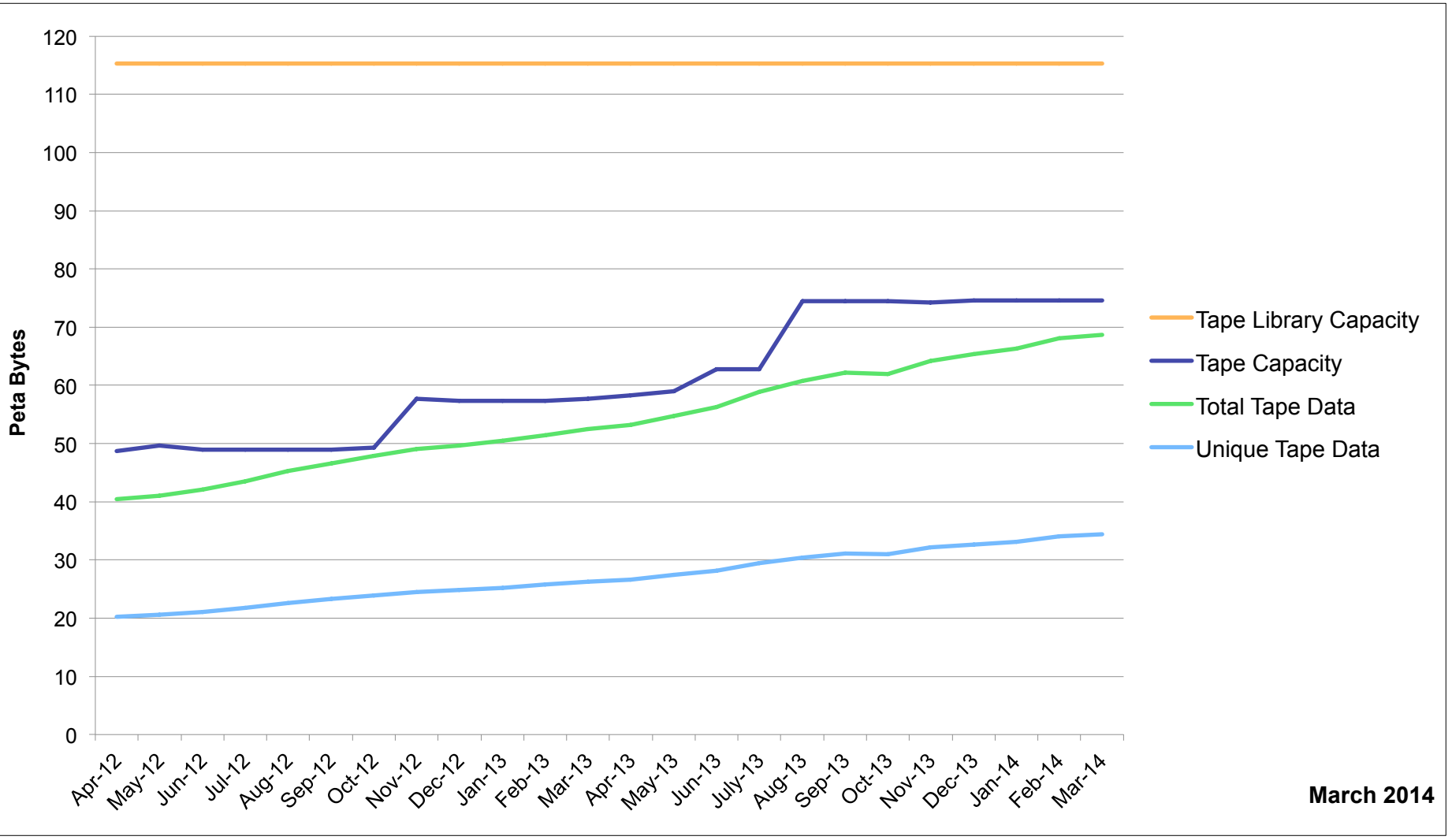


① 24 Sandy Bridge Racks added
② Columbia 21, 23, and 24 retired, Endeavour 2 added
③ Columbia 22 retired; Endeavour 1 added
④ 32 Harpertown Racks retired
⑤ 32 Harpertown Racks retired; 46 Ivy Bridge Racks added
⑥ 6 Ivy Bridge Racks added; 20 Nehalem and 12 Westmere Racks Retired
⑦ 8 Ivy Bridge Racks added mid-Feb; 8 additional Ivy Bridge Racks late Feb.
⑧ 4 Ivy Bridge Racks added mid-March

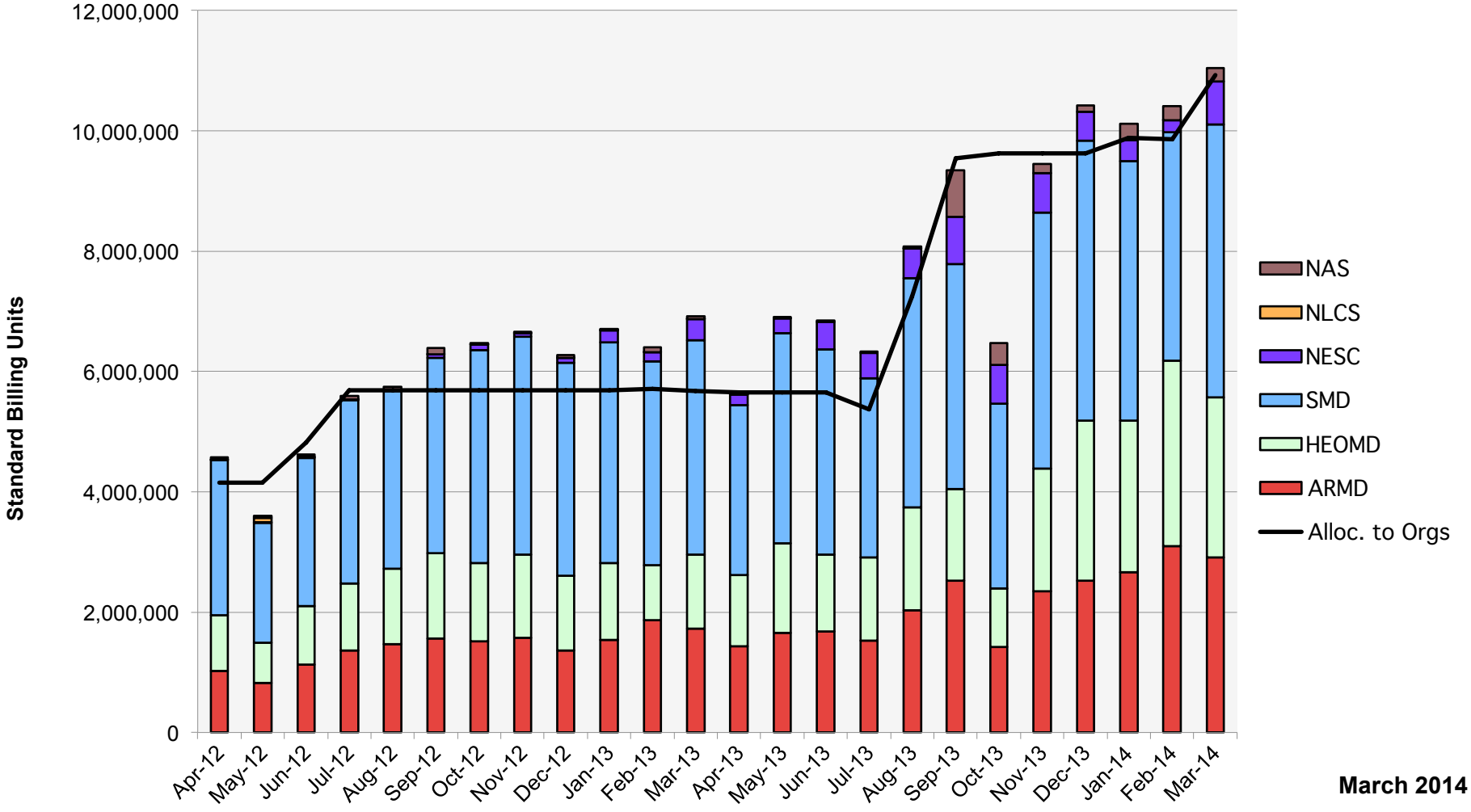
Tape Archive Status



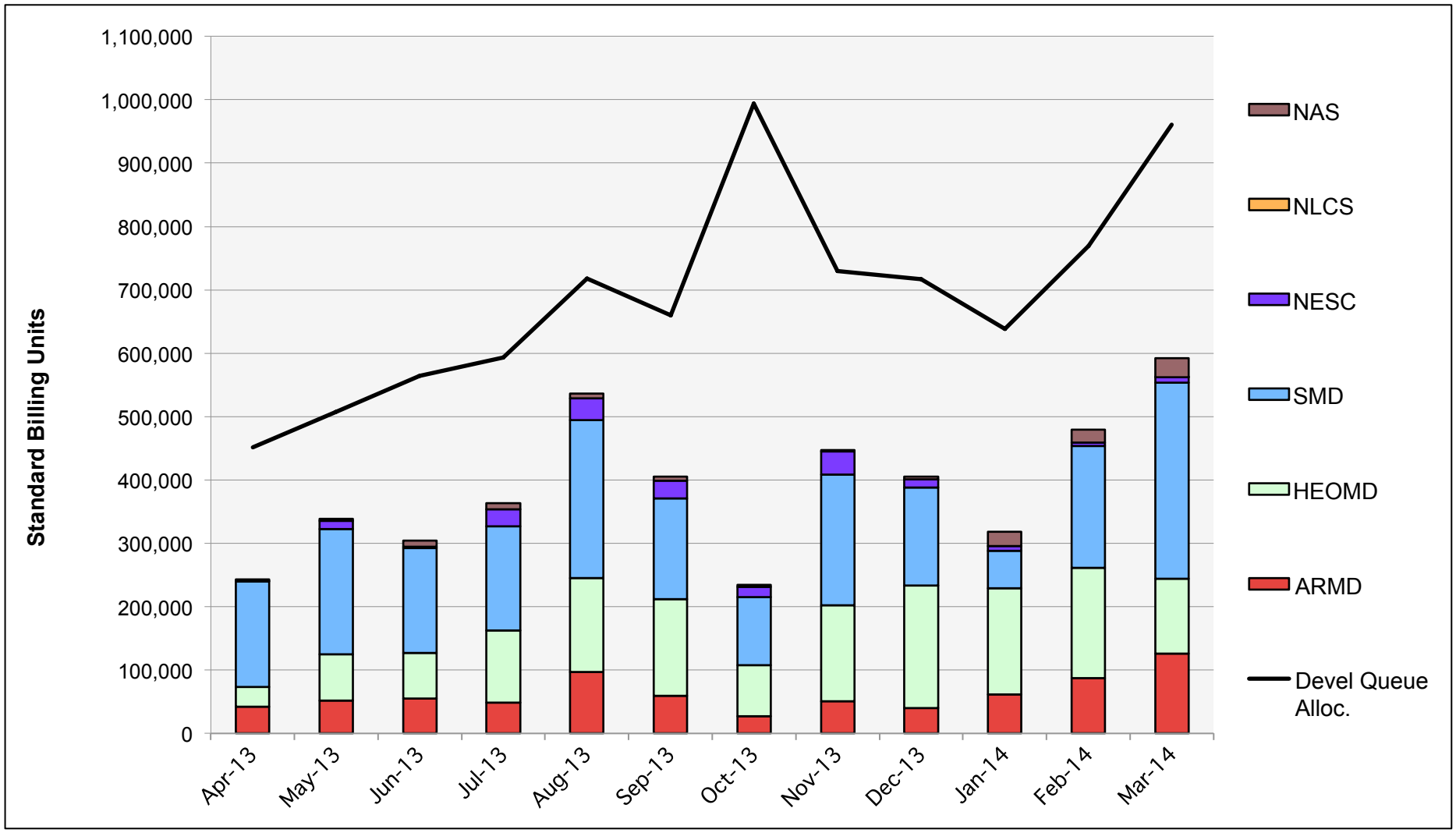
Tape Archive Status



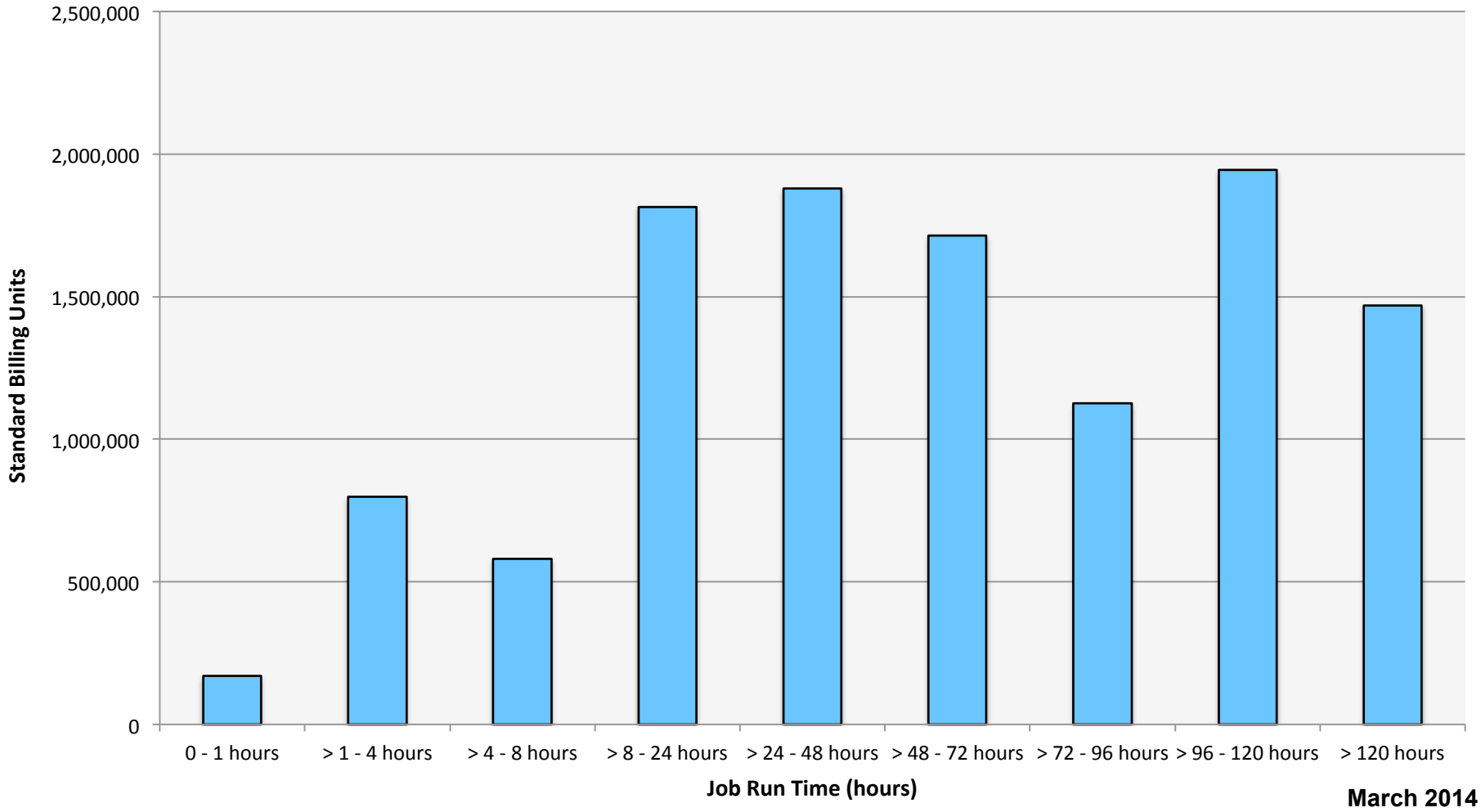
Pleiades:
SBUs Reported, Normalized to 30-Day Month



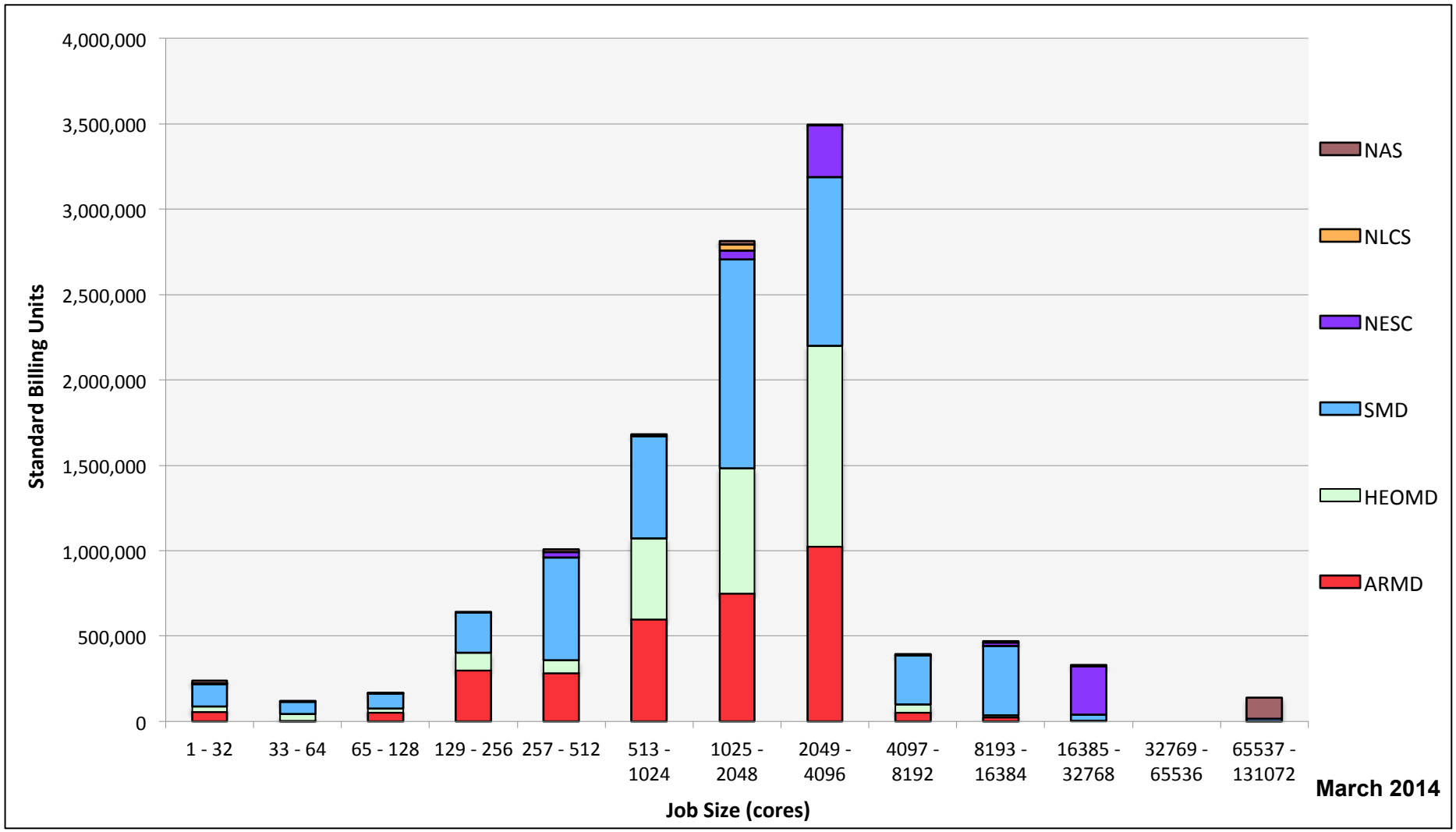
Pleiades:
Devel Queue Utilization



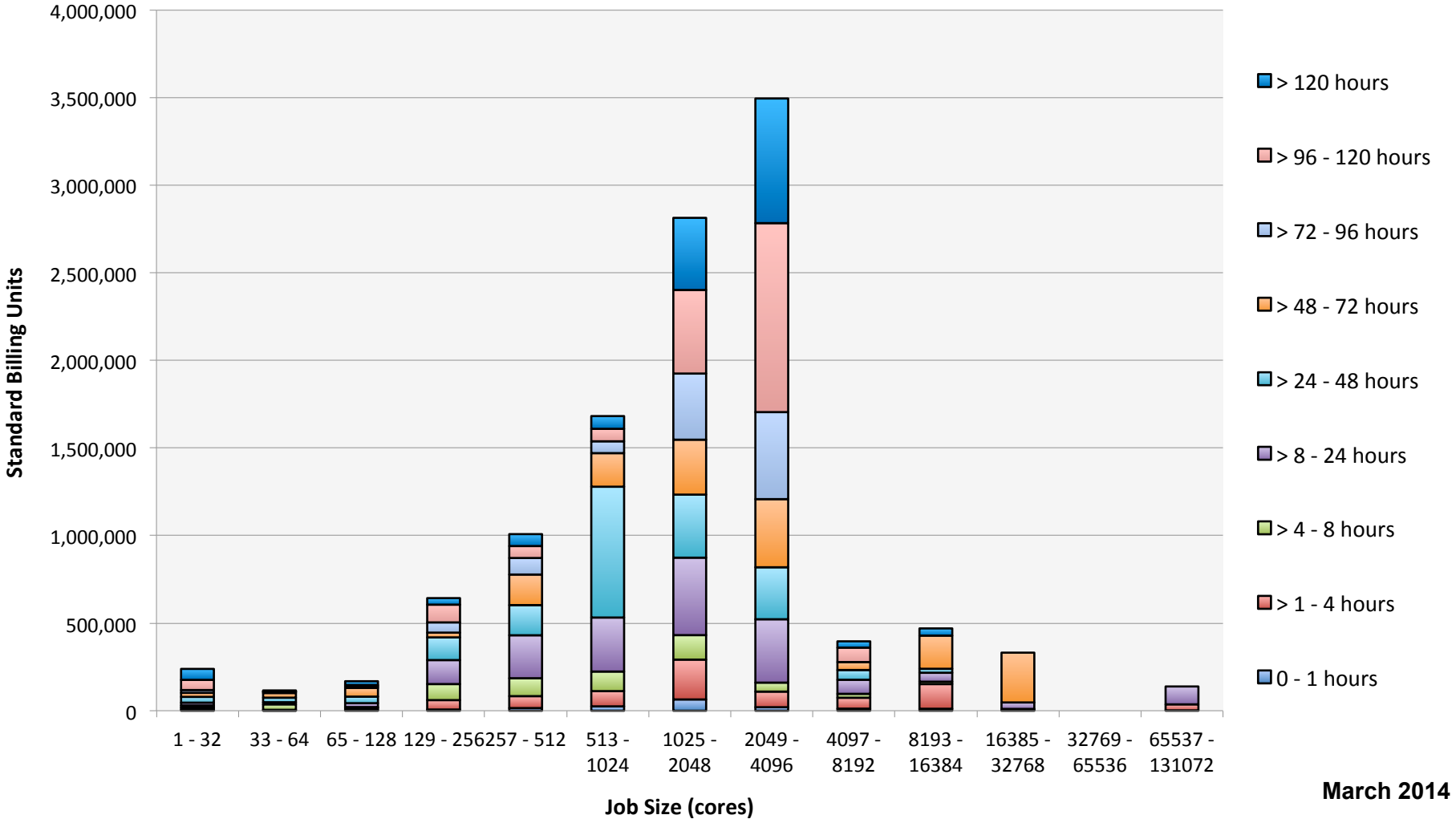
Pleiades:
Monthly Utilization by Job Length



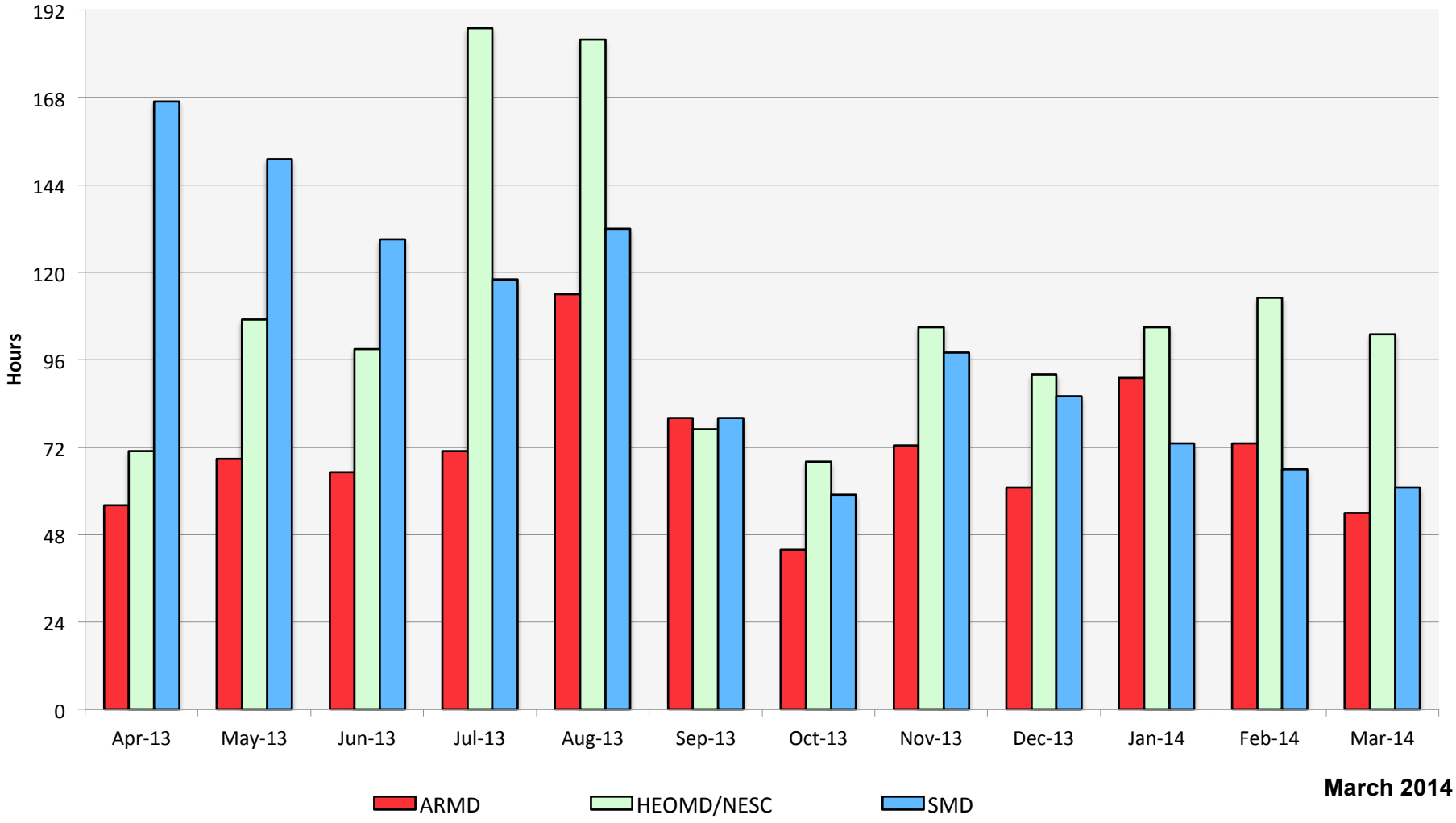
Pleiades:
Monthly Utilization by Size and Mission



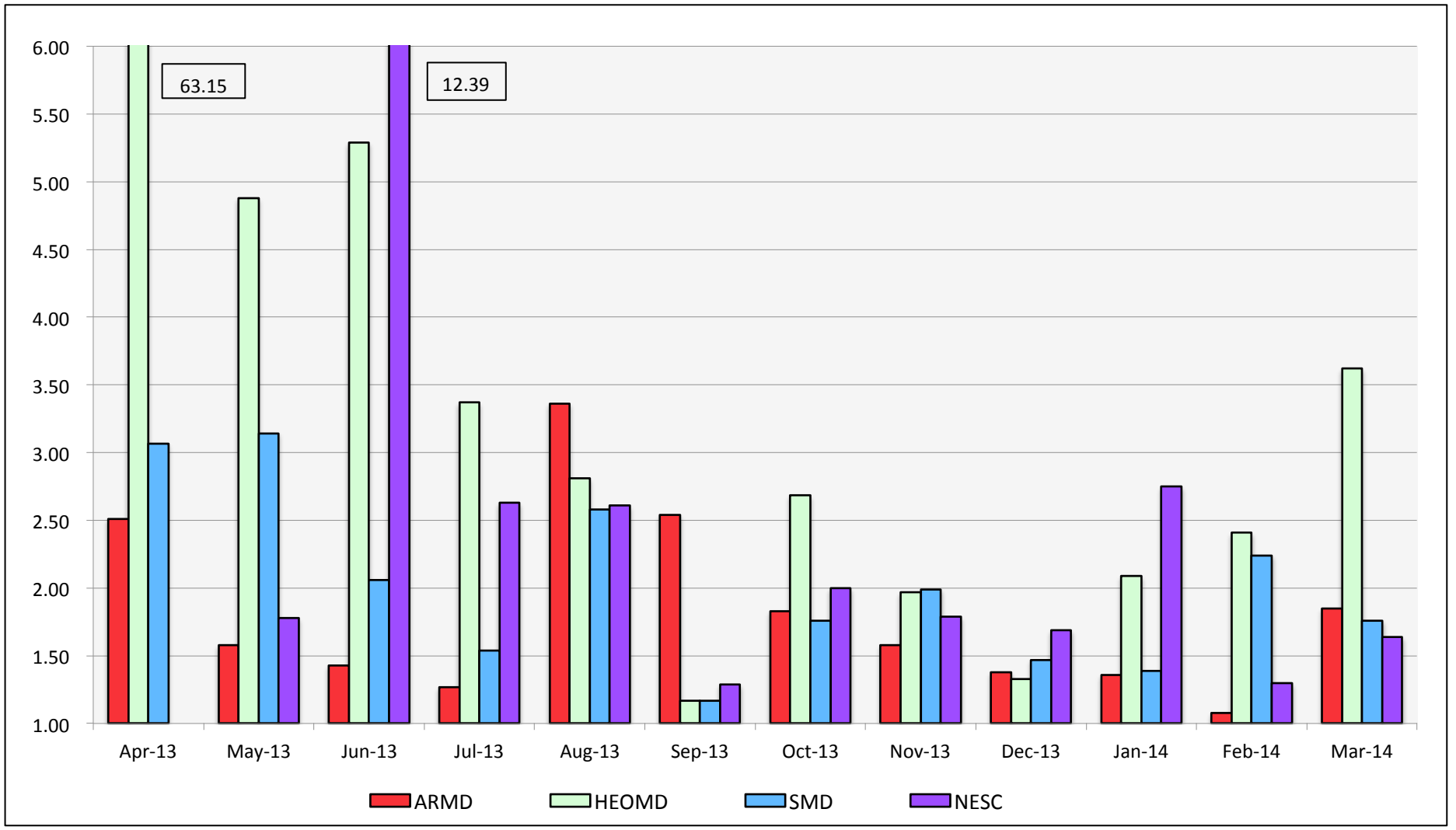
Pleiades:
Monthly Utilization by Size and Length



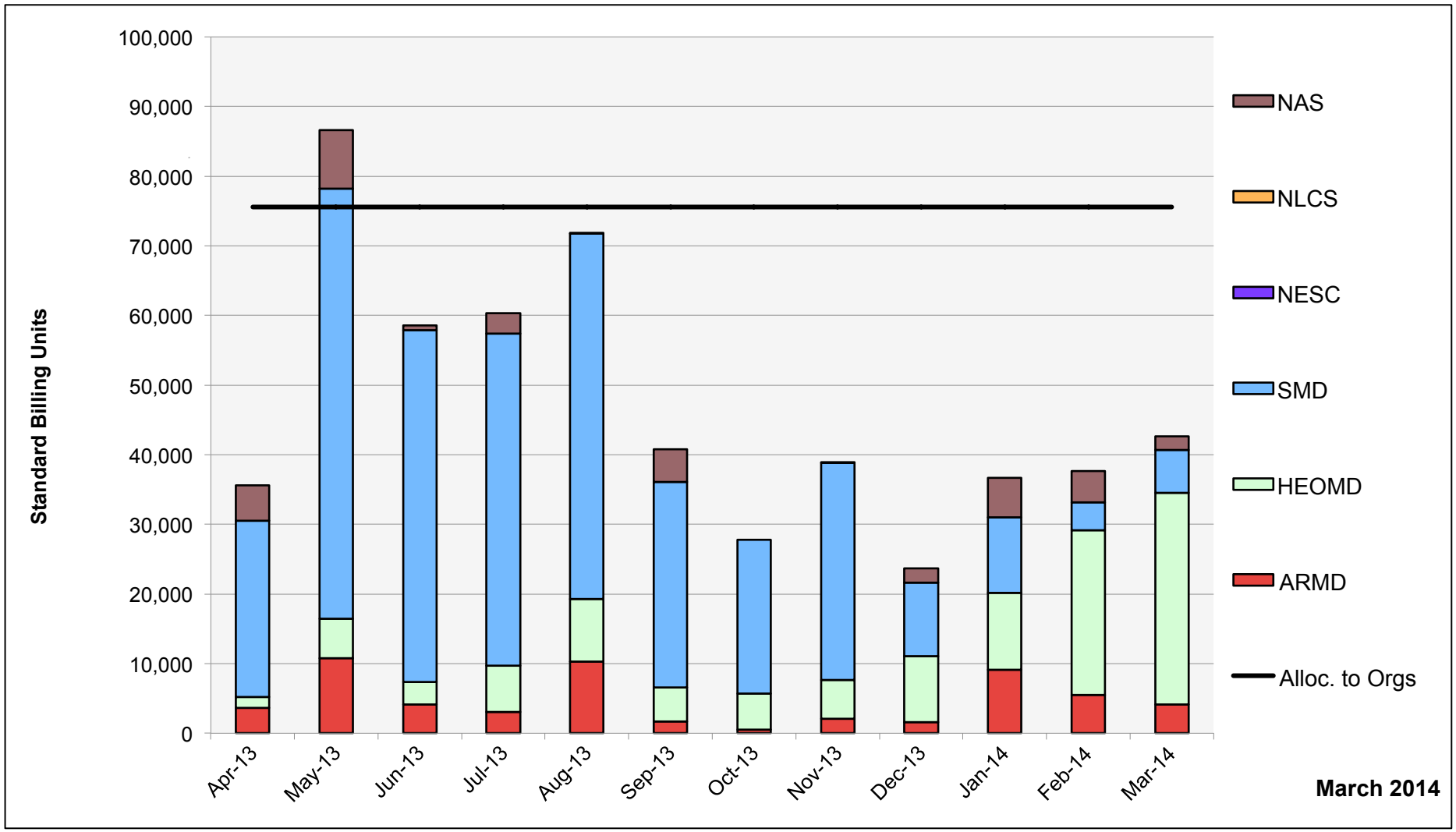
Pleiades:
Average Time to Clear All Jobs



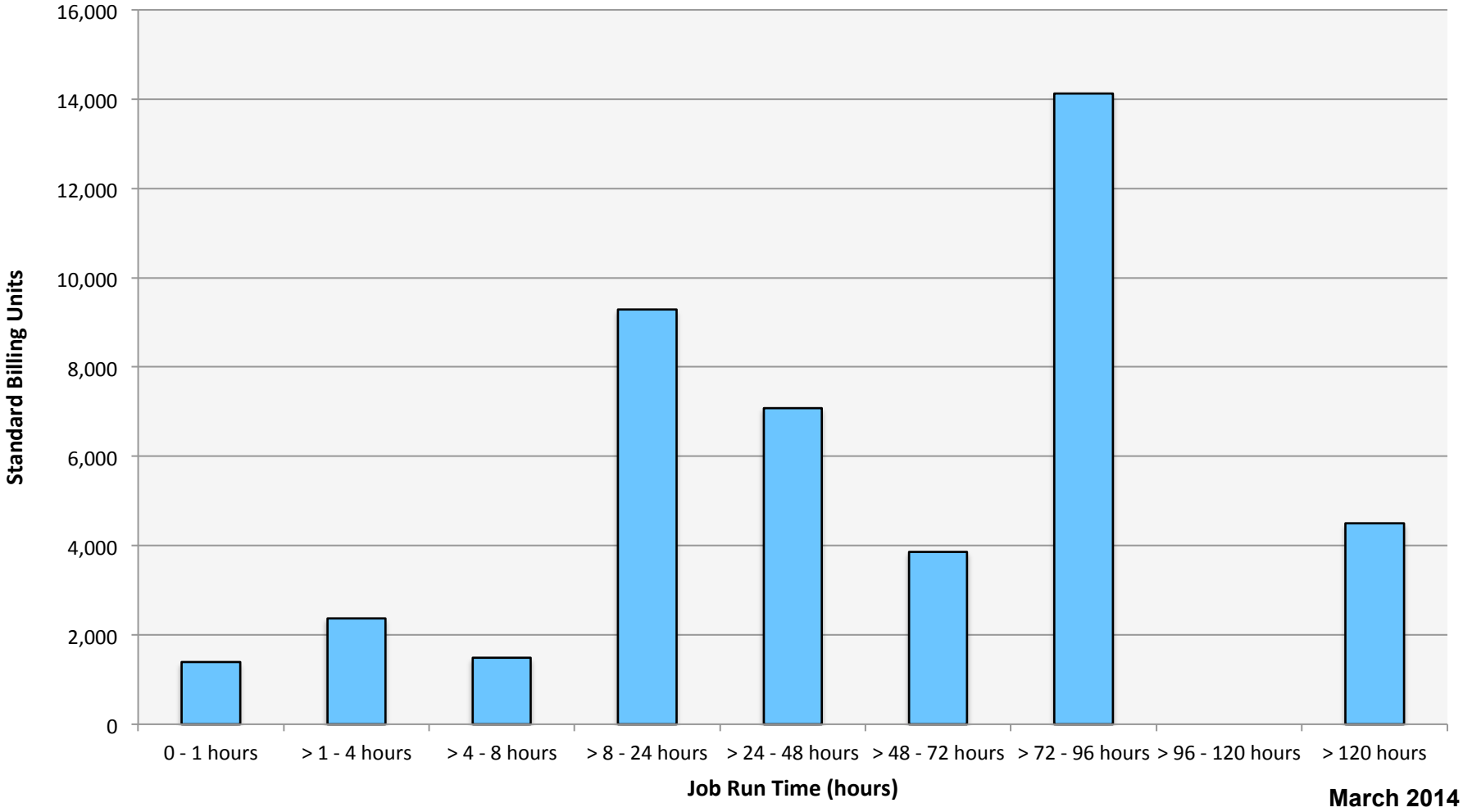
Pleiades:
Average Expansion Factor



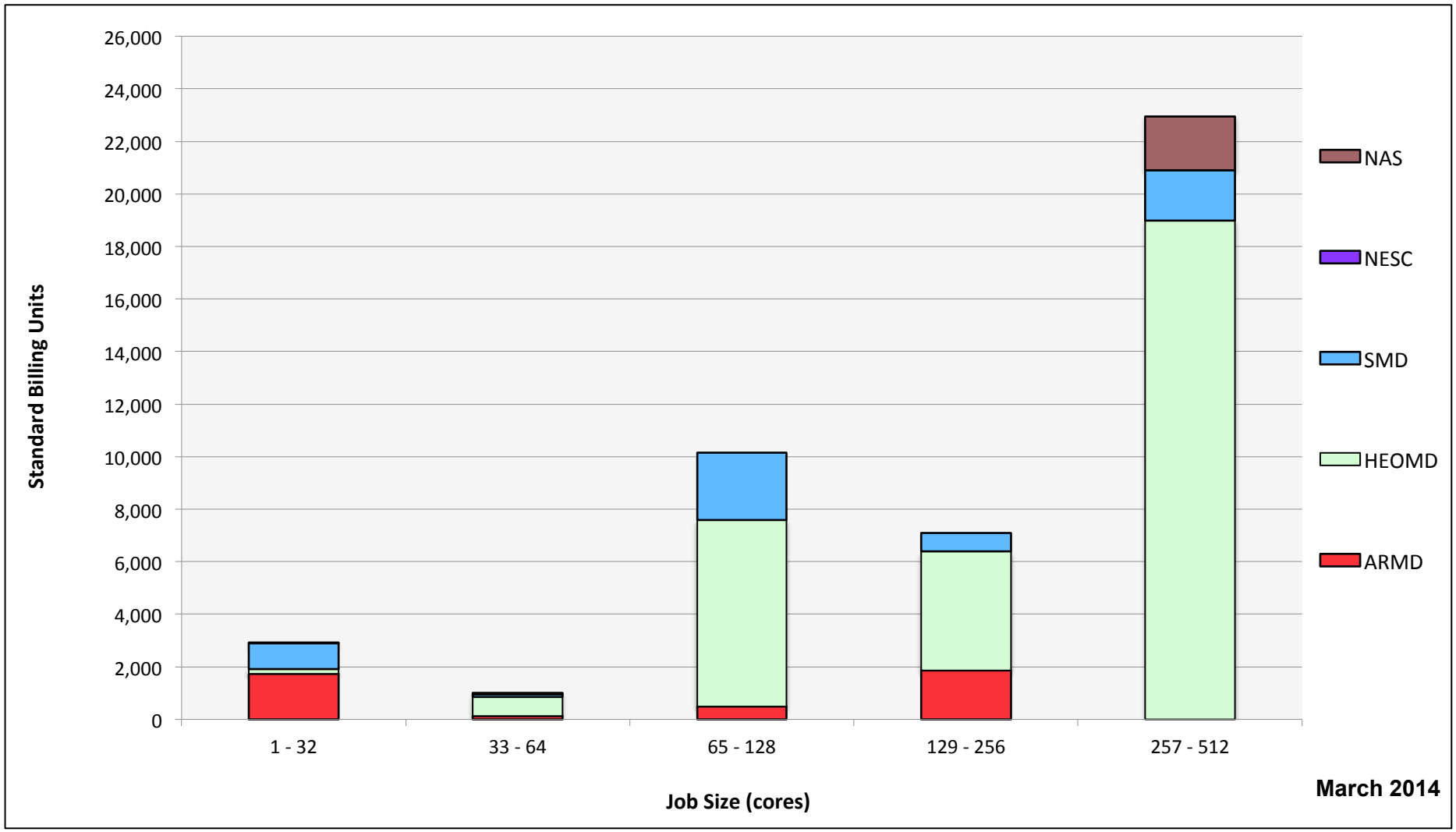
Endeavour:
SBUs Reported, Normalized to 30-Day Month



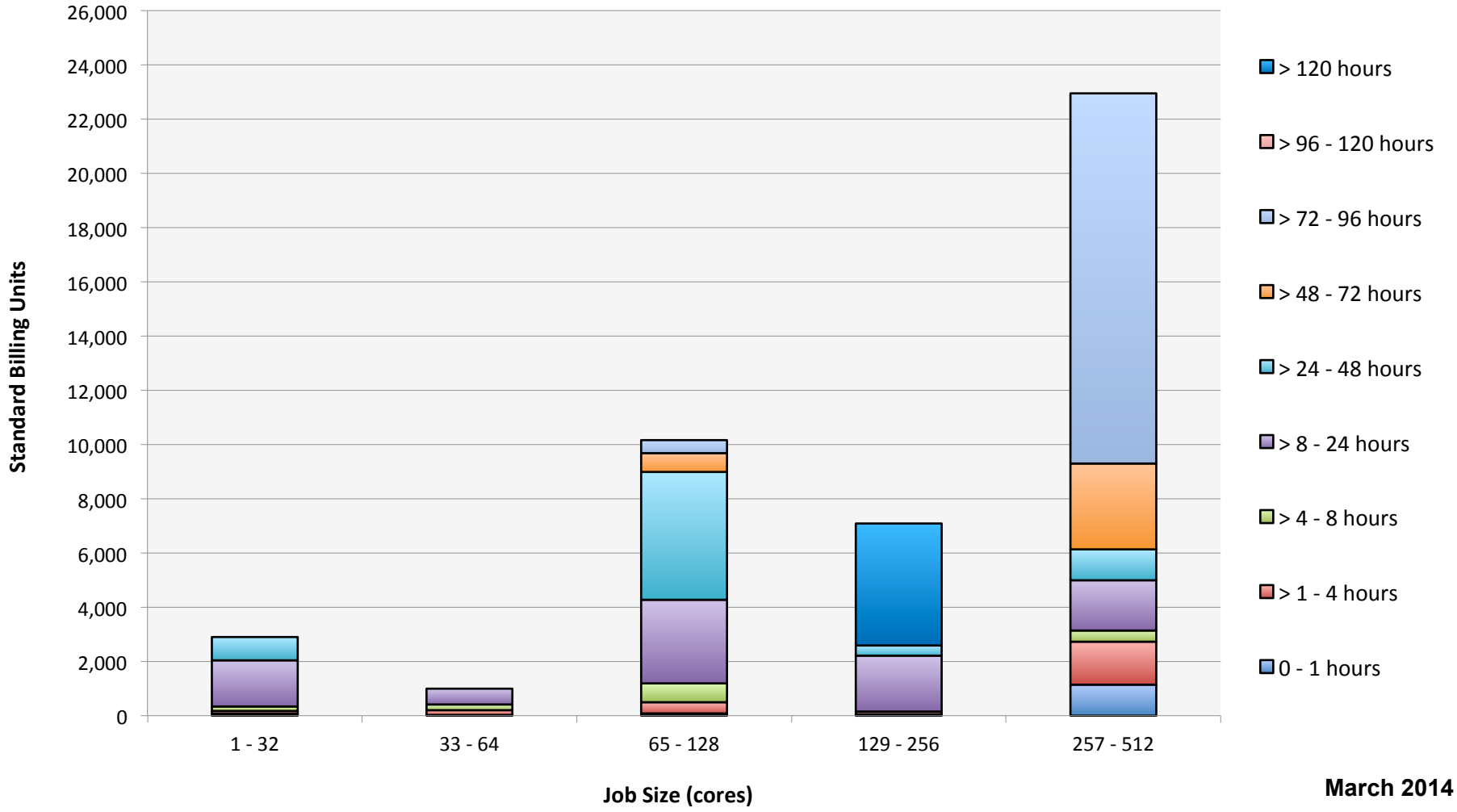
Endeavour:
Monthly Utilization by Job Length



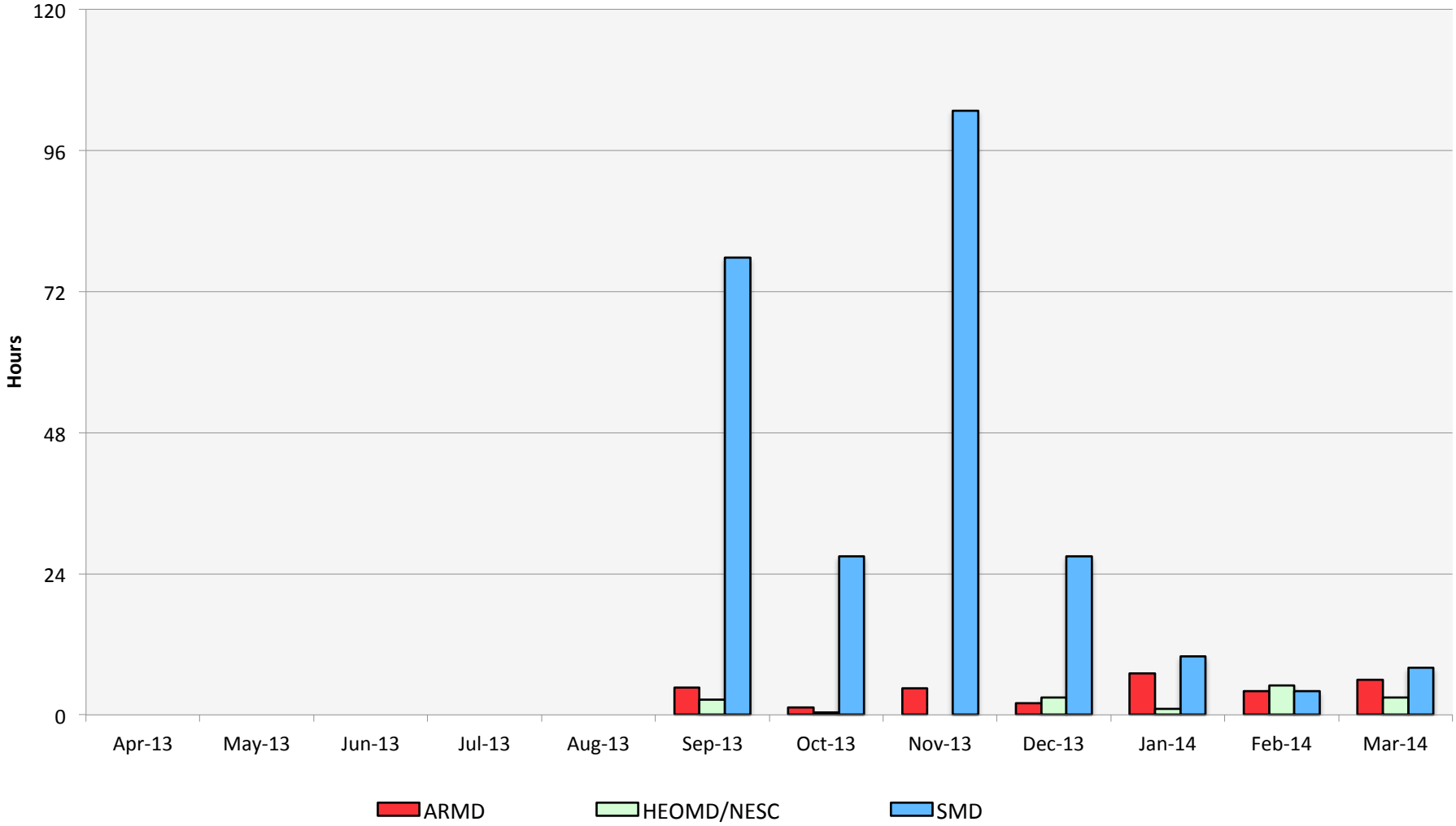
Endeavour:
Monthly Utilization by Size and Mission



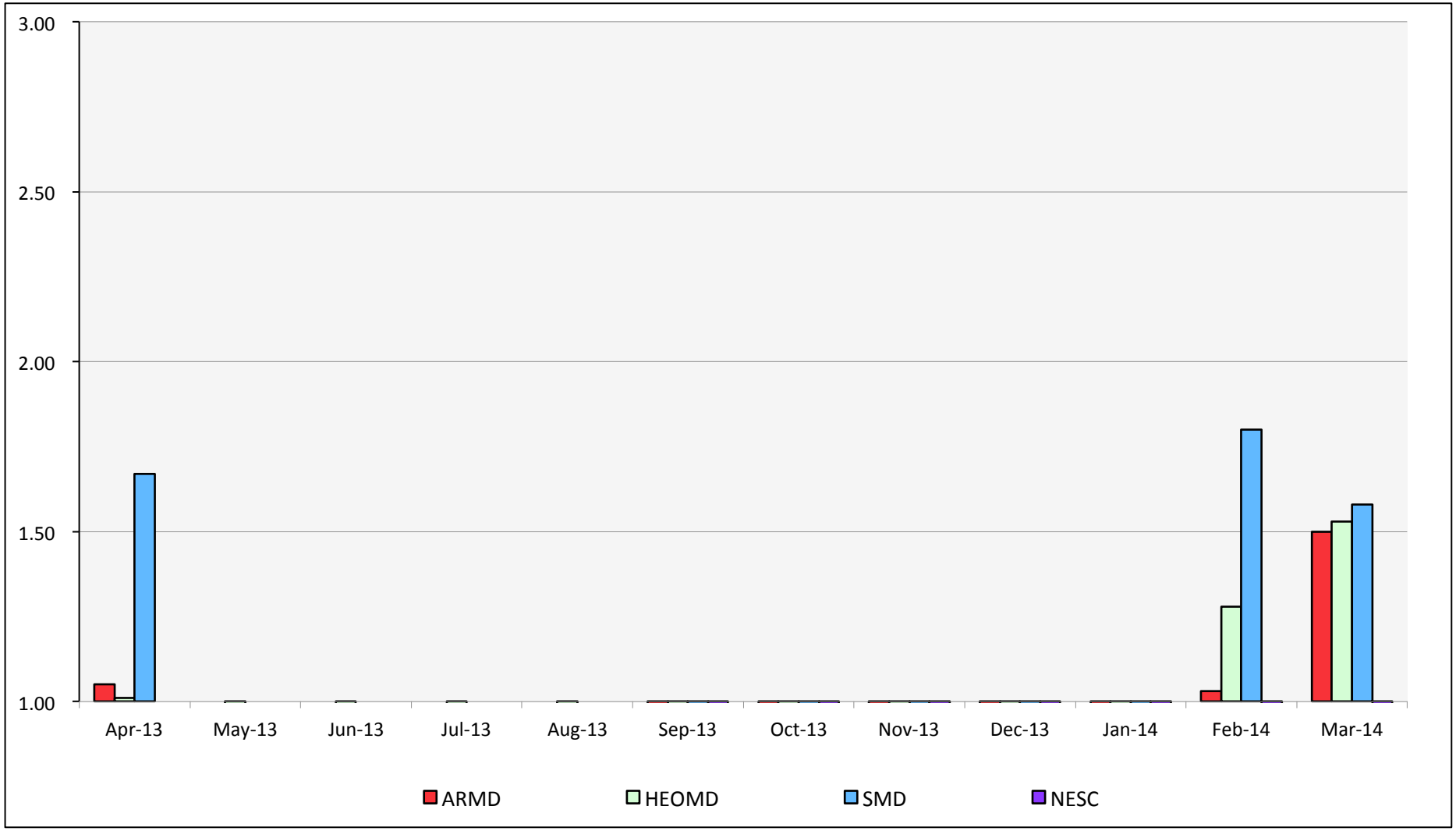
Endeavour:
Monthly Utilization by Size and Length



Endeavour:
Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor



Maia:
SBUs Reported, Normalized to 30-Day Month